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Probabilities of Diagonal and Non-Diagonal Couplings between *d* Electrons in Transition Metal II. The *d*-Band-Center-Shift Energy

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Abstract

It is shown that the full account of the non-diagonal couplings between *d* electrons sited on different atoms in a transition metal implemented in the framework of the Wills-Harrison model leads not only to vanishing the *d*-band term in the internal energy but to vanishing the whole *d*-electron-depended part of the internal energy.

Keywords: Transition metal, Wills-Harrison model, *d*-state coupling

The *d*-band energy considered in the previous paper (henceforth referred to as I) is not the single contribution due to *d* electrons to the transition-metal internal energy in the Wills-Harrison (WH) model [1]. The second *d*-electron-depended WH energy contribution is the energy arisen because of the shift in the center of gravity of the *d* band due to nonorthogonality of *d*-like states, E_c (hereafter, per atom in atomic units):

$$E_c = \frac{z_d}{2N} \sum_{m=1}^{N} \sum_{\substack{l=1 \\ l \neq m}}^{N} V_c(\vec{r}_{ml}) \quad , \tag{1}$$

where z_d is the effective *d*-electron valence, N - number of atoms,

$$V_c(r) = \frac{r_d^6}{r^8} K_c \quad , \tag{2}$$

where r_d is the *d*-state radius, K_c - combinatoric coefficient, which as well as the coefficient K_b (paper I) in the WH approximation depends on diagonal only couplings between *d* electrons sited on different atoms:

$$K_c^{\mathrm{WH}} = -2\sum_{m=-2}^{2}\frac{y_m x_m}{5} \quad , \tag{3}$$

where *m* is the magnet quantum number, $y_m = y_{|m|}$,

$$y_0 = -45/\pi\,,\quad y_1 = 30/\pi\,,\quad y_2 = -15/2\pi \quad , \tag{4}$$

$$x_m = x_{|m|} = -\frac{1}{8}\left(1+\frac{4m^2-1}{9}\right)y_m \quad , \tag{5}$$

From (3)-(5)

$$K_c^{\mathrm{WH}} = 225/\pi^2 \quad . \tag{6}$$

Taking into account the probability *p* that all 25 *d*-*d* couplings between two different atoms in metal are equiprobable, the coefficient K_c is expressed as follows [2]:

$$K_c = -\frac{2}{5}\left[\left(1-\frac{4p}{5}\right)y_0x_0 + \left(2-\frac{6p}{5}\right)(y_1x_1+y_2x_2) + \right.$$
$$\left. + \frac{2p}{5}(y_0(x_1+x_2)+x_0(y_1+y_2)) + \frac{4p}{5}(y_1x_2+y_2x_1)\right] \quad . \tag{7}$$

If now to apply (4) and (5) to (7), the result will be similar to one obtained in the paper I:

$$K_c = K_c^{\mathrm{WH}}(1-p)\,. \tag{8}$$

It denotes that at $p=1$ not only the *d*-band energy, E_b, is equal to zero, but also E_c and, consequently, the whole *d*-electron-depended part of the internal energy in the WH model, which is equal to $E_b + E_c$.

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